Ethane

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 1.04

Global applicability domain: Inside

Local applicability domain index: 9.06e-01

Confidence level: 6.03e-01

Nearest Neighbors from the Training Set

Image not found
Ethane
Measured: 0.42
Predicted: 1.04

Image not found
Chloromethane
Measured: 1.39
Predicted: 1.58

Image not found
Dimethyl ether
Measured: 1.37
Predicted: 1.58

Image not found
Ethylene
Measured: 0.28
Predicted: 4.19e-01

Image not found
Nitromethane
Measured: 2.53
Predicted: 1.63